

A Parametric Equation of State for the Liquid-Liquid Critical Point in Supercooled Water

D.A. Fuentevilla^S and M.A. Anisimov^C

*Department of Chemical & Biomolecular Engineering and Institute for Physical Science & Technology,
University of Maryland, College Park, MD, U.S.A.
anisimov@umd.edu*

We have developed a scaled parametric equation of state to describe and predict thermodynamic properties of water in supercooled conditions. The equation of state is built on the assumption that in the supercooled water an additional critical point, the critical point of liquid-liquid separation, exists. Although this second critical point of water is not accessible experimentally, the near-critical anomalies do affect thermodynamic and transport properties of water in the metastable and even in the stable regions, and can be observed experimentally. Our approach is based on the principle of critical-point universality. The equation of state is universal in terms of theoretical scaling fields and belongs to the three-dimensional Ising-model class of universality. The theoretical scaling fields are postulated to be analytical combinations of physical fields (pressure and temperature). The proposed equation of state enables us to accurately locate the “Widom line” (the locus of stability minima) and the position of the critical point, as well as to predict the thermodynamic properties in the regions that may not be accessible to direct experiments.